

# Computational Study on Epoxidation of Propylene by Dioxygen Using the Silanol-Functionalized Polyoxometalates-Supported Osmium Oxide Catalyst

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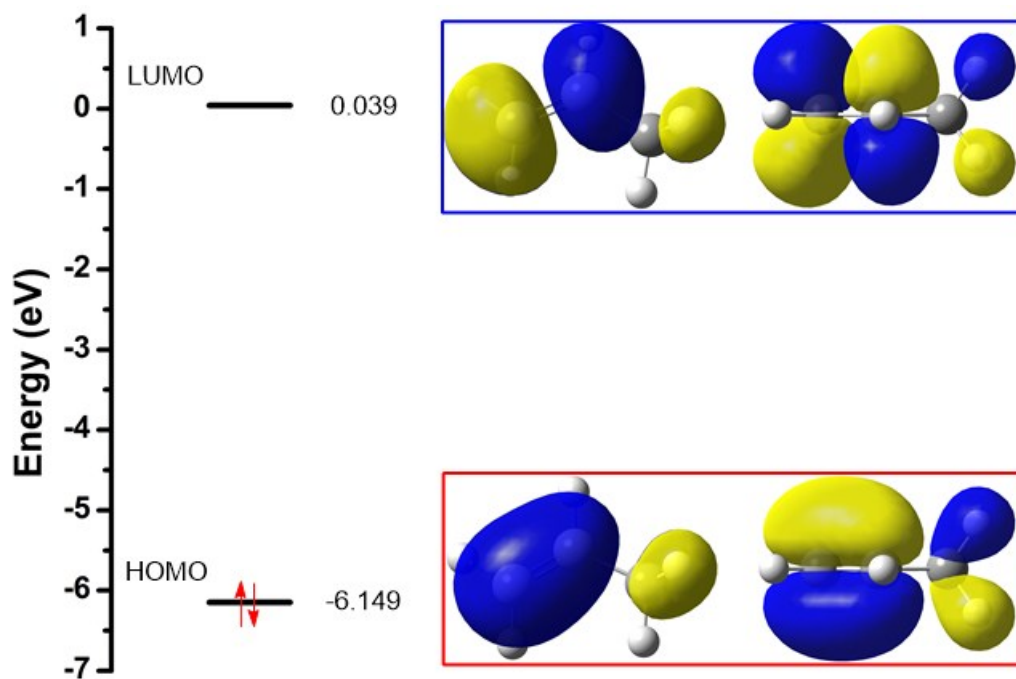
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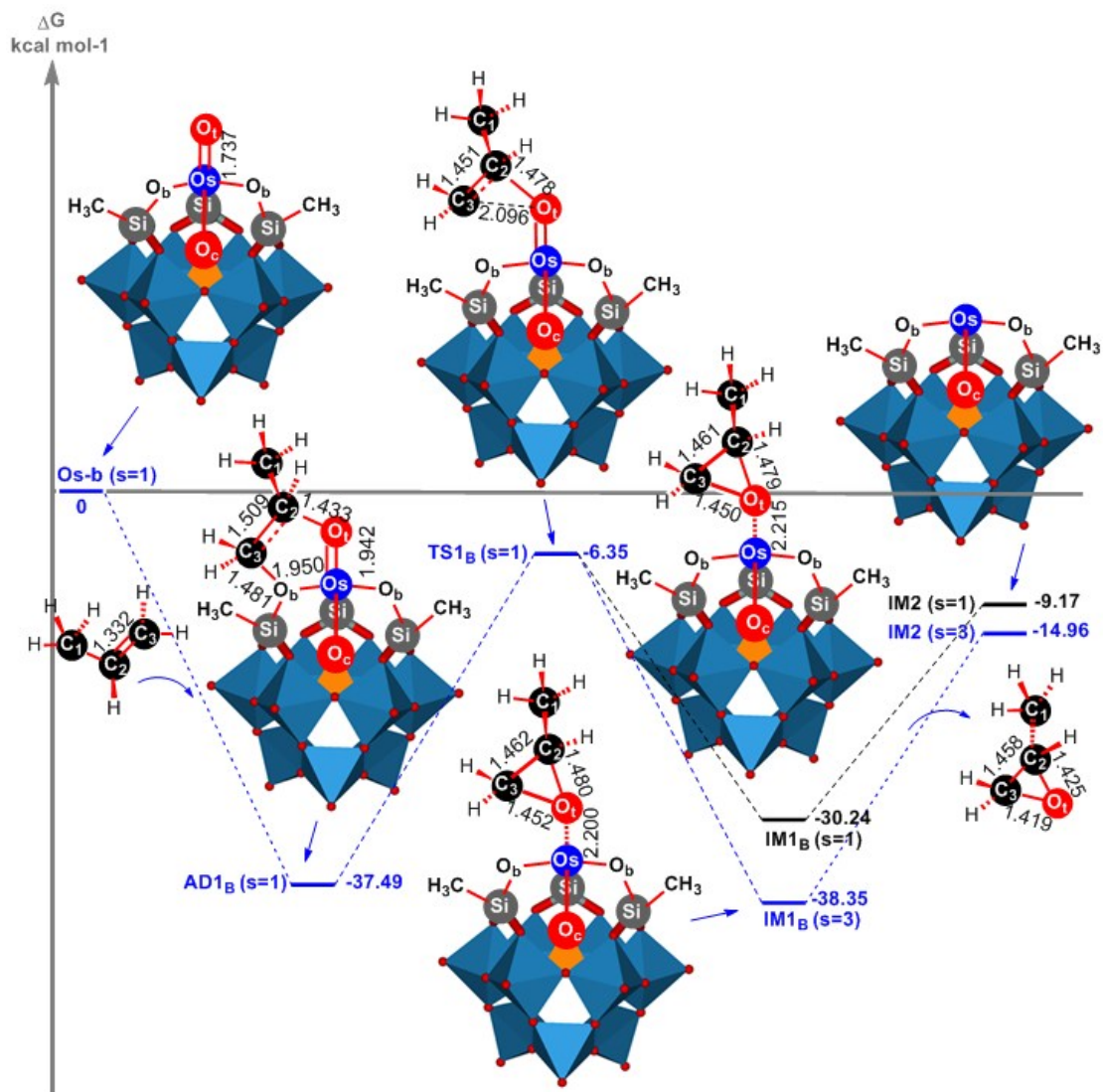
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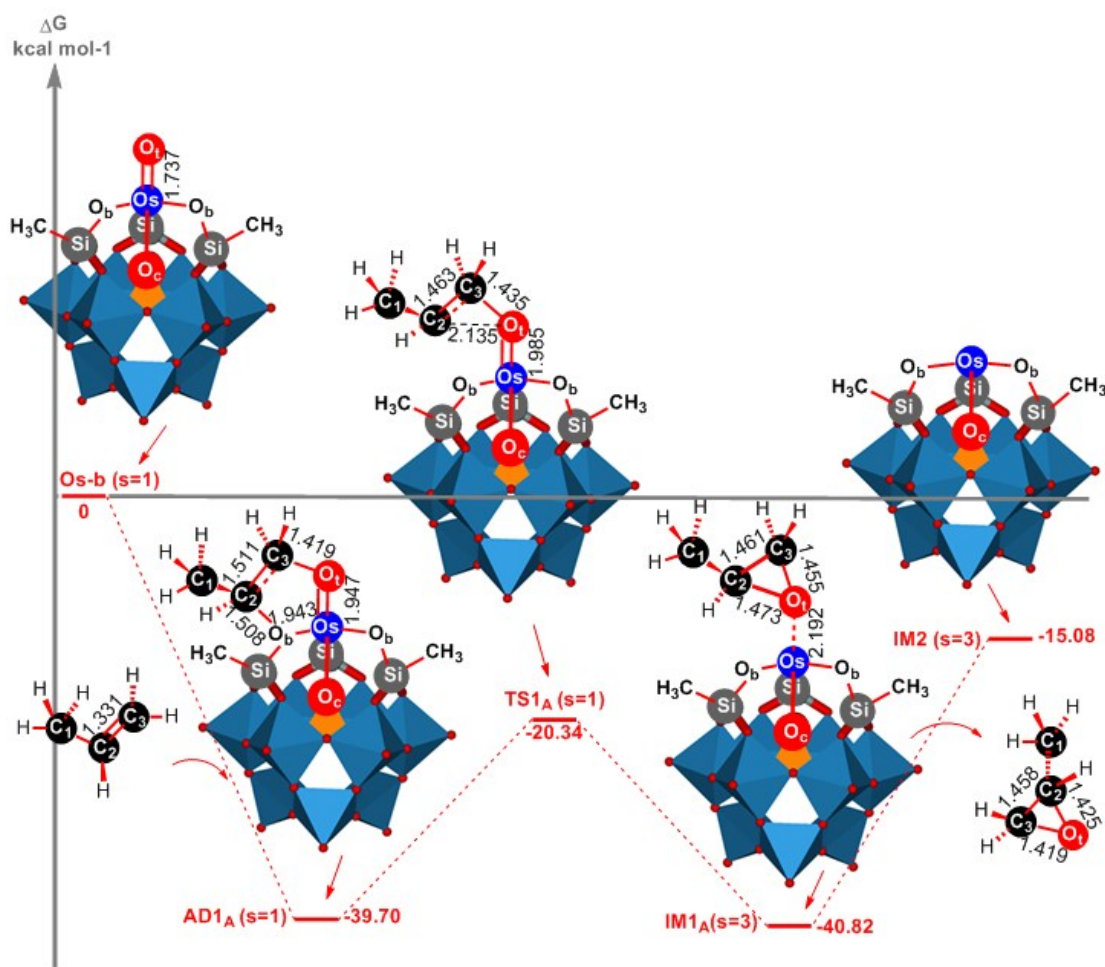
Electronic supplementary information (ESI) available. See DOI: XXXXXXXXXXXX



**Fig. S1** The frontier molecular orbitals of propylene molecule



**Fig. S2** The calculated free energy profile for the first oxygen transfer step with bond lengths in angstrom and relative energy in kcal mol<sup>-1</sup>



**Fig. S3** The relative energy obtained by fully optimizing each structure of the optimal reaction path in Fig. 5 with larger basis sets

In order to obtain a more accurate energy value and to test the reliability of our computational method, we fully optimize each structure of the optimal reaction path in Figure 5 using a large basis set. The 6-31G(d,p) basis set was used for all non-metal atoms. The base set used for the metal atom is unchanged. The refined energy is shown in Figure S3. The research results show that the energy value and the intermediates and transition states geometric configuration do not change significantly after increasing the basis sets, which also verifies the correctness of our method.

**Os-a**

W	3.12385700	-1.36818900	-1.42462300
W	0.16604400	-0.67905700	-3.57416800
W	-0.01620000	-3.34151900	-1.02376800
Si	-2.80869700	-3.36436900	0.68556000
P	0.06743800	0.07855100	-0.03015500
O	4.28569200	-2.24865000	-2.28896200
O	0.38777600	-1.33068300	-5.12644700
O	0.18052100	-4.86750200	-1.74527700
O	3.82721800	0.40814600	-1.41737700
O	1.87606500	-0.83999600	-2.82557200
O	1.74146400	-2.68296000	-1.03143200
O	-0.38012000	-2.18097000	-2.50457100
O	0.09925000	-3.74525200	0.85653200
O	-1.81197100	-0.24649000	-3.74253900
O	-2.01695800	-3.48036800	-0.70022200
O	1.63035200	0.00064500	0.00959400
O	-0.61153900	-1.28610100	0.24975600
O	-3.86886500	-1.80938100	0.20086800
O	-5.31056000	0.53926000	-0.27420800
C	-4.20593800	-4.52831800	0.94683800
W	3.06711300	-0.62014800	1.91491800
W	-0.11361100	-2.52177700	2.34266600
W	0.09177300	0.98607000	3.48176300
Si	-2.66599100	2.35502900	2.45508200
O	4.19171700	-1.03388400	3.11399000
O	0.01574900	-3.56741400	3.67501300
O	0.34453900	1.07733400	5.15731900
O	3.74238700	-1.55276800	0.38507600
O	1.66977900	-1.95324100	2.11108500
O	1.79345500	0.48841900	2.88572500
O	-0.48235000	-0.83072400	3.15216500
O	0.32877100	2.78746200	2.86204500
O	-2.09706300	-2.78892500	2.00011800
O	-1.86298200	1.49788600	3.53344000
O	-0.41979700	1.10659400	1.02009100
O	-3.13001600	0.74450400	1.44208300
C	-4.38201400	2.86944600	2.87840900
W	3.18244100	1.91622700	-0.40045400
W	0.10656800	3.42967200	1.05094000
W	0.22239100	2.61906200	-2.54906900
Si	-2.56780900	1.04695900	-3.19126000
O	4.40118900	3.06692300	-0.64610100
O	0.26811200	5.10542900	1.28656100

O	0.45597700	4.01706300	-3.48561500
O	3.79018000	0.99810600	1.16851200
O	1.87256200	2.88496600	0.64805400
O	1.93447600	2.29192700	-1.85591400
O	-0.26808400	3.31233700	-0.82038500
O	0.41517400	1.21284500	-3.85671500
O	-1.90157900	3.29451000	1.41372100
O	-1.77585800	2.39377100	-2.87919000
O	-0.30088400	0.53286400	-1.48578400
O	-2.73868900	0.38863200	-1.36243700
C	-4.33983900	1.22235400	-3.65741400
H	-4.34158800	3.74300900	3.53855800
H	-4.94696400	3.16119000	1.98760300
H	-4.91591300	2.07425900	3.40601300
H	-4.39378400	1.52808700	-4.70830400
H	-4.88054700	0.27546500	-3.56654400
H	-4.84546000	1.99202400	-3.06727400
H	-3.81133700	-5.51823100	1.20098800
H	-4.84347400	-4.20047000	1.77277100
H	-4.80798100	-4.62975200	0.03949500
Os	-3.72921000	-0.06385500	0.00927600

**Os-b**

W	-0.06523400	1.88461800	2.94538900
W	-2.97406500	2.05578600	0.65500400
W	0.29328300	3.55306200	-0.21752700
Si	1.10649400	2.64654200	-3.29963000
P	-0.12620500	0.00416100	-0.52958000
O	-0.17126700	2.75012800	4.39818400
O	-4.09730800	3.20582700	1.19296300
O	0.28193900	5.24909400	-0.28711300
O	-0.52804800	0.09991500	3.44592800
O	-1.80642400	1.96192900	2.15397900
O	0.39306700	3.25908100	1.65078300
O	-1.57122600	3.09234600	-0.14103000
O	2.19705000	3.19404800	-0.50027000
O	-3.75779500	1.71747300	-1.13753800
O	0.07608500	3.11756900	-2.15779200
O	0.71487800	1.18633400	-0.03774600
O	0.06220800	-0.03666400	-2.14876500
O	0.08792800	1.47154900	-4.27590000
O	-1.84784100	0.06898100	-5.30740400
C	1.51272600	3.84143600	-4.63755900
W	2.79507900	-0.23364300	2.20753300

W	3.11764400	1.56255300	-0.91925700
W	2.77215000	-2.15161800	-0.86088600
Si	0.57978800	-2.89129400	-3.20894500
O	4.07895300	-0.33341600	3.30731700
O	4.68344400	2.07828200	-1.31992500
O	4.21279800	-2.96288100	-1.24064200
O	1.71243900	1.20801300	2.87344700
O	3.40160500	1.02074300	0.88060200
O	3.16439800	-1.61507100	0.92249600
O	3.05421500	-0.31031000	-1.30511600
O	1.55776700	-3.56129400	-0.39534400
O	2.30895600	1.73787000	-2.74400200
O	1.94136600	-2.22576300	-2.67427900
O	0.47754100	-1.29457600	0.01110300
O	-0.18917300	-1.57832100	-4.21548000
C	0.74355300	-4.19834000	-4.49275600
W	-0.41746200	-1.75632200	2.99900600
W	-0.37940500	-3.54640200	-0.11029500
W	-3.30918400	-1.43445100	0.71120400
Si	-3.94933000	0.34836900	-1.96682600
O	-0.66266300	-2.54373400	4.47890600
O	-0.71034500	-5.21175300	-0.14158900
O	-4.63889000	-2.33283400	1.25754600
O	1.46240200	-1.41377000	2.90890100
O	-0.20961400	-3.22467800	1.75089700
O	-2.15375400	-1.54487600	2.22823400
O	-2.11889100	-2.74336500	-0.03809700
O	-3.77472200	0.37279800	1.16825700
O	-0.51872900	-3.11280300	-2.05368900
O	-3.97787900	-1.01592300	-1.11132200
O	-1.62114800	0.15218100	-0.23379500
O	-2.34426100	0.24617500	-2.79700100
C	-5.11456800	0.42271100	-3.38808700
H	1.19273400	-5.09281900	-4.04754000
H	-0.23422100	-4.47477300	-4.89809600
H	1.38675500	-3.86760100	-5.31331800
H	-4.93416000	1.31162000	-3.99987600
H	-5.02186100	-0.46561400	-4.02028700
H	-6.14514000	0.46813000	-3.01983800
H	2.12900100	4.65050000	-4.23078900
H	2.07498600	3.35532100	-5.43994900
H	0.60382500	4.28242300	-5.05727700
Os	-0.91522800	0.03509100	-3.84234500

**AD1<sub>A</sub>**

W	-3.12729900	0.54194300	1.47640700
W	-0.32911600	2.75685500	2.45473500
W	-0.48901700	-0.79373000	3.47195700
Si	2.45114700	-2.19253100	2.85554600
P	0.49688700	0.07491800	0.13128700
O	-4.65693100	0.89537600	2.11268700
O	-0.76194700	3.80813700	3.71445400
O	-0.71279400	-1.04877600	5.13732000
O	-3.16313600	1.33901600	-0.25908200
O	-2.02659900	2.02293600	1.98364700
O	-2.26786000	-0.41245700	2.92092500
O	-0.08365700	1.06981900	3.35002000
O	-0.57839800	-2.63423600	2.80914900
O	1.63655200	3.05748700	2.48632500
O	1.48813300	-1.00243300	3.34847100
O	-0.38425000	-0.77177200	1.06572200
O	1.98560300	-0.51548800	0.15561200
O	3.78003300	-1.27010500	2.01786000
O	5.65841100	0.42753600	1.11806600
C	3.43385600	-3.07284900	4.13778000
W	-2.70161600	-2.06375800	-1.00356500
W	-0.07727200	-3.39067400	1.12700000
W	0.60485200	-2.52042200	-2.42664000
Si	3.40952100	-0.89352200	-2.50874300
O	-3.98963100	-3.05170300	-1.48891600
O	-0.14593100	-5.06318700	1.40695700
O	0.77483700	-3.87318300	-3.43708400
O	-3.37967900	-1.08641600	0.48988900
O	-1.75692400	-3.13857500	0.28084800
O	-1.27667300	-2.50147100	-2.22896500
O	0.65057200	-3.17729200	-0.63991500
O	0.70307000	-1.02725300	-3.62405700
O	1.81175400	-3.09451500	1.69039700
O	2.57406500	-2.19352200	-2.11358600
O	-0.01610500	-0.13093000	-1.30871500
O	4.50079400	-0.57705400	-0.96716000
C	4.68533600	-1.14727200	-3.81893100
W	-2.46941900	1.38166600	-2.03761700
W	0.80411900	0.90840000	-3.31557000
W	0.24885600	3.61654100	-0.87557600
Si	2.68136500	3.32444800	1.28872900
O	-3.71073100	2.10862700	-2.93220600
O	1.25310100	1.41832800	-4.87480000



O	0.13231800	5.14899200	-1.59396900
O	-2.91526700	-0.47105700	-2.05436100
O	-1.07368400	1.14372700	-3.36810800
O	-1.40210400	2.84882300	-1.40117000
O	0.97250900	2.49674000	-2.27630800
O	-0.39005500	3.91941800	0.91623600
O	2.62822700	0.50381100	-2.55010400
O	2.07122400	3.82360400	-0.11662200
O	0.56028300	1.56338000	0.51607800
O	3.31480700	1.70109300	0.77997800
C	4.24455000	4.15073700	1.80360200
H	5.28688500	-0.25557000	-4.01989400
H	5.34025900	-2.00520100	-3.63619400
H	4.12956600	-1.36688100	-4.73939700
H	4.03782900	5.17831600	2.12052200
H	4.71068000	3.62683500	2.64367300
H	4.95690600	4.19046500	0.97372200
H	3.95784800	-2.36436300	4.78632000
H	2.76737000	-3.67516500	4.76425300
H	4.16807700	-3.74624800	3.68553000
Os	3.79589200	-0.00434900	0.75016700
C	5.99981500	-0.73147800	-0.95794200
C	6.47509000	0.37161200	-0.04029700
H	6.30112900	-0.55526900	-1.99450700
H	7.50982200	0.20131700	0.28034400
H	6.43037700	1.34995100	-0.54506100
C	6.30841900	-2.13206000	-0.50012200
H	6.01784300	-2.27898100	0.54706000
H	5.78559600	-2.87434100	-1.11192300
H	7.38477500	-2.31797700	-0.58032100

**AD1<sub>B</sub>**

W	-1.94424600	1.58327400	-2.47732400
W	1.18008700	0.12435500	-3.26648900
W	1.14456600	3.24855000	-1.30952600
Si	3.20716600	2.69068100	1.16372000
P	0.34659900	-0.03138400	0.18765800
O	-2.89004000	2.44841200	-3.58521500
O	1.90131000	0.23788000	-4.80308700
O	1.49833700	4.63175100	-2.22695400
O	-2.86192800	-0.08868300	-2.31884500
O	-0.55670200	0.80586800	-3.59384200
O	-0.59443600	2.84445400	-1.93735600
O	1.66716700	1.77576200	-2.44759700

O	0.45012500	3.98332100	0.33727300
O	2.74808000	-0.56799600	-2.19207000
O	2.88188700	3.11539700	-0.35784200
O	0.76942800	1.44178400	0.33278600
O	1.58889500	-0.97797200	0.53395400
O	3.37171700	0.91097500	0.94245000
O	5.33014100	-0.72739000	1.66665900
C	4.88354100	3.15318800	1.77263800
W	-3.09268700	1.46151000	1.02381500
W	0.07218600	3.10475000	2.00682100
W	-1.06380500	-0.09239000	3.46785900
Si	1.42859400	-2.28177600	3.39166600
O	-4.52955700	2.28366200	1.38298600
O	-0.17321400	4.41894900	3.05166600
O	-1.45521300	-0.03901100	5.12100700
O	-2.72815300	1.96043600	-0.79050800
O	-1.70504100	2.71773900	1.46044500
O	-2.66481600	0.60072300	2.69657400
O	-0.19700500	1.56657800	3.16047200
O	-1.57748600	-1.95119500	3.04091600
O	2.03179400	2.89616900	2.24791400
O	0.79079200	-0.81583200	3.57081200
O	-0.82331800	-0.41291000	1.11359200
O	3.03445700	-1.86138800	2.61068900
C	2.02303900	-3.14840100	4.90109800
W	-3.15676500	-1.49636200	-1.05881600
W	-1.17306700	-3.06645000	1.55698300
W	0.01934700	-2.97078900	-1.97025500
Si	3.14108700	-2.09988400	-1.93033700
O	-4.61576200	-2.19987700	-1.55563800
O	-1.70855800	-4.60359200	2.03587100
O	-0.06916900	-4.47206600	-2.75736100
O	-3.68628200	-0.16851400	0.21589200
O	-2.63324200	-2.54143400	0.46985200
O	-1.80686200	-2.47456800	-2.03077400
O	-0.25600800	-3.30702800	-0.12381200
O	0.61651500	-1.74917600	-3.33069900
O	0.67842300	-3.18599900	2.29713600
O	1.97451900	-3.08445200	-1.47471700
O	-0.07412100	-0.36774500	-1.25930900
O	4.13253800	-1.86943400	-0.30940100
C	4.42521300	-2.79015800	-3.05953600
H	2.58250300	-4.05283100	4.64454100
H	2.66034300	-2.49799200	5.50719700

H	1.16478200	-3.44718400	5.51244400
H	5.26000200	-2.10083700	-3.22605300
H	4.80420400	-3.77028900	-2.75466900
H	3.93394500	-2.92535200	-4.03152900
H	5.18816500	2.51513500	2.60871600
H	5.62651600	3.06861100	0.97435700
H	4.88023500	4.18972100	2.12539300
Os	3.44839300	-0.84317100	1.20143300
C	5.54131600	-2.28294700	-0.11321300
C	6.21022100	-1.14264000	0.61464700
H	5.50580800	-3.20596800	0.47431700
H	5.95568800	-2.48193700	-1.10343500
H	7.12344600	-1.50445300	1.10521800
C	6.52140100	0.04208500	-0.28374500
H	6.90595300	0.87408900	0.31239400
H	7.28135300	-0.22693200	-1.02566600
H	5.62653200	0.38803700	-0.81886300

#### AD1c

W	0.01228000	1.87050200	2.99420500
W	-2.88803900	2.22404200	0.72462800
W	0.43498100	3.62313700	-0.09476700
Si	1.19823900	2.78681100	-3.21592000
P	-0.13004600	0.12728800	-0.52941700
O	-0.06933300	2.67114900	4.48534400
O	-3.97470900	3.39674900	1.29143900
O	0.48843900	5.32031900	-0.12343800
O	-0.51741800	0.08003400	3.41871700
O	-1.73345300	2.04076100	2.22365000
O	0.51803000	3.28651200	1.77352000
O	-1.44928900	3.24274800	-0.02546300
O	2.31978500	3.19990000	-0.38004500
O	-3.65853200	1.97771000	-1.09422600
O	0.19651800	3.23912000	-2.03651900
O	0.74744000	1.23030600	0.07746300
O	0.06046200	0.19241200	-2.13443000
O	0.16331800	1.70454100	-4.24091600
O	-1.86201500	0.45271900	-5.30595100
C	1.64858600	4.05390200	-4.47319500
W	2.79137200	-0.31520900	2.17786400
W	3.18893400	1.56344400	-0.88530300
W	2.66822600	-2.12970500	-0.95470400
Si	0.45934800	-2.66098300	-3.33297800
O	4.07455500	-0.52156800	3.26466600

O	4.77732700	2.03149400	-1.25536000
O	4.07442400	-2.98607100	-1.36776400
O	1.76893800	1.12874100	2.92091700
O	3.45283500	0.94891400	0.90372700
O	3.08213400	-1.67196800	0.84067200
O	3.04952900	-0.28320900	-1.32798900
O	1.40682000	-3.51731200	-0.55718100
O	2.39811100	1.85194200	-2.69196100
O	1.83699100	-2.06699800	-2.76750700
O	0.41855600	-1.23367300	-0.08428800
O	-0.29629600	-1.32494800	-4.30120600
C	0.64781200	-3.93758800	-4.65441400
W	-0.46650200	-1.75863900	2.91277300
W	-0.52950800	-3.42856700	-0.26810600
W	-3.36783800	-1.24841600	0.67103000
Si	-3.93443700	0.63791200	-1.94071500
O	-0.73461400	-2.59050700	4.36484600
O	-0.92947700	-5.07831200	-0.34902500
O	-4.72495500	-2.11936600	1.19842600
O	1.41667400	-1.48623600	2.83376900
O	-0.33920800	-3.18217800	1.60260800
O	-2.20853900	-1.45924000	2.16126100
O	-2.23887400	-2.56657800	-0.16316700
O	-3.76381600	0.56143700	1.18360800
O	-0.65379500	-2.95353100	-2.20804500
O	-4.06401500	-0.74588200	-1.12540700
O	-1.62345100	0.30429800	-0.22618000
O	-2.38063800	0.34089500	-2.79768200
C	-5.11188900	0.82412600	-3.34841600
H	1.19838700	-4.78798100	-4.23619600
H	-0.31343900	-4.31647800	-5.01601700
H	1.22599700	-3.55687200	-5.50232400
H	-5.26780400	-0.13318000	-3.85658400
H	-6.08303900	1.17008300	-2.97891300
H	-4.75250500	1.55748300	-4.07744100
H	2.28182100	4.81929200	-4.01187800
H	2.20704500	3.60579700	-5.30027300
H	0.75765000	4.54576400	-4.87473500
Os	-0.92504800	0.31303800	-3.82798700
C	-1.79551900	-1.83561800	-6.65855800
C	-2.91804900	-1.75445900	-5.89861100
H	-1.00798300	-2.55143000	-6.43353400
H	-1.66433600	-1.20924700	-7.53658700
H	-3.69651000	-1.05684600	-6.21305400

C	-3.18260000	-2.54739800	-4.67949600
H	-4.15371600	-3.05553300	-4.74727600
H	-2.40647700	-3.29124700	-4.47587500
H	-3.25928800	-1.90705200	-3.78482300

**TS1<sub>A</sub>**

W	-3.16191200	0.70682300	1.54503700
W	-0.19873800	2.73818500	2.43365700
W	-0.56044800	-0.79553400	3.45599700
Si	2.24356400	-2.40484700	2.76623300
P	0.33275400	0.01414200	0.08419900
O	-4.64859600	1.16720100	2.21463000
O	-0.50660900	3.81782800	3.70650700
O	-0.71281000	-1.04755600	5.13047200
O	-3.17757400	1.49708900	-0.18391000
O	-1.95134200	2.11684400	2.02982200
O	-2.32658400	-0.28998900	2.98740100
O	-0.02712800	1.03974700	3.32122100
O	-0.78253800	-2.62054600	2.79751500
O	1.78633500	2.89936100	2.37655500
O	1.40368500	-1.11012800	3.22478600
O	-0.57582300	-0.76088800	1.04555300
O	1.78589000	-0.69616600	0.08870900
O	3.61516800	-1.61953600	1.85742200
O	5.49666000	0.08291200	1.08461600
C	3.14359800	-3.34395700	4.06593000
W	-2.99802700	-1.93464400	-0.92945600
W	-0.40685400	-3.43629400	1.09793900
W	0.22941700	-2.58565600	-2.47804300
Si	3.18715500	-1.13782600	-2.45313400
O	-4.37525600	-2.81755000	-1.37246000
O	-0.56122800	-5.10125300	1.39220100
O	0.27579100	-3.94309500	-3.49489700
O	-3.54982800	-0.90811400	0.58907800
O	-2.10488400	-3.07947700	0.33841100
O	-1.65280200	-2.47364500	-2.18795200
O	0.26669100	-3.25809800	-0.67325800
O	0.33553000	-1.10518900	-3.67504900
O	1.51988300	-3.25711100	1.61390800
O	2.18023300	-2.37000600	-2.20655300
O	-0.20417900	-0.17394300	-1.34207000
O	4.20586400	-0.88914400	-1.00980400
C	4.51981600	-1.49135500	-3.68965700
W	-2.56237700	1.49346500	-2.00160000

W	0.64440600	0.81048500	-3.36750600
W	0.30188900	3.57298900	-0.93141700
Si	2.78631600	3.09481000	1.12840100
O	-3.79633300	2.28601400	-2.85049200
O	1.06436300	1.30075600	-4.94004000
O	0.25744700	5.10989700	-1.64870900
O	-3.12562100	-0.32589500	-1.97073200
O	-1.23298100	1.18013400	-3.35941500
O	-1.40770500	2.91635900	-1.39937100
O	0.91679300	2.39225200	-2.33188600
O	-0.23844500	3.89798000	0.88971900
O	2.41655200	0.26936900	-2.66388500
O	2.16223400	3.67042400	-0.23971100
O	0.54512700	1.48841500	0.45468100
O	3.28056600	1.45032000	0.57136500
C	4.42664700	3.80601500	1.58880300
H	5.18113200	-0.63200900	-3.84353900
H	5.11936000	-2.36185600	-3.40338400
H	4.05412500	-1.71891900	-4.65500000
H	4.28657400	4.78488200	2.05918500
H	4.95140100	3.16668200	2.30687000
H	5.05734000	3.94880100	0.70566300
H	3.76363700	-2.67857400	4.67425900
H	2.42336100	-3.83247900	4.73092900
H	3.77854300	-4.12056600	3.62956400
Os	3.60065100	-0.30246500	0.64261000
C	6.77951300	-0.40377900	-0.55259100
C	6.37323500	0.78698300	0.19368700
H	6.38099500	-0.56893500	-1.55088800
H	7.16255400	1.26065900	0.78851500
H	5.83788800	1.53898500	-0.39941500
C	7.60626600	-1.44700100	0.03925700
H	7.91000200	-1.23528900	1.06664100
H	7.10176800	-2.42310800	-0.00675400
H	8.50092900	-1.57553900	-0.59355100

**TS1<sub>B</sub>**

W	-1.96433500	1.64677900	-2.44968900
W	1.11132600	0.09479200	-3.32823600
W	1.20130200	3.20911700	-1.34295800
Si	3.28682300	2.54991000	1.08133800
P	0.31940100	-0.05082100	0.14245100
O	-2.90469300	2.55070100	-3.53130200
O	1.77729100	0.22317300	-4.88700300

O	1.56992700	4.59243300	-2.25440400
O	-2.93048900	0.00905000	-2.26956700
O	-0.62206700	0.85182500	-3.58614600
O	-0.56664300	2.86389700	-1.90830600
O	1.65389600	1.73411300	-2.50035000
O	0.57425700	3.93870500	0.34079500
O	2.64493200	-0.67985100	-2.32806200
O	2.95578900	3.02218000	-0.42465000
O	0.82754100	1.38946200	0.29610000
O	1.55026000	-1.04191900	0.48367800
O	3.44545300	0.77642700	0.80040300
O	5.28406400	-0.96492300	1.61105400
C	4.96163300	3.02172100	1.70826000
W	-3.04566700	1.53890900	1.07621300
W	0.19358500	3.06520200	2.00786200
W	-1.01081600	-0.11435900	3.45695800
Si	1.40372900	-2.37899900	3.31583000
O	-4.44910400	2.39976200	1.47590800
O	0.02610500	4.37594500	3.07215800
O	-1.35001000	-0.07633700	5.12217300
O	-2.70227500	2.03961100	-0.73531500
O	-1.60694600	2.74715100	1.49860600
O	-2.60190600	0.64485800	2.73326000
O	-0.09977400	1.52192600	3.14734400
O	-1.57446900	-1.94576800	3.01690500
O	2.14732800	2.75729800	2.20135100
O	0.83759000	-0.88090400	3.48569400
O	-0.83970400	-0.40292300	1.08311900
O	3.00531300	-2.04219200	2.49064600
C	1.96445000	-3.26631600	4.82541500
W	-3.25690200	-1.40583100	-1.01839100
W	-1.25503300	-3.07175000	1.50547500
W	-0.13958600	-2.95641300	-2.05425800
Si	3.05375700	-2.18363000	-1.89463500
O	-4.75118000	-2.04892100	-1.49362900
O	-1.81440300	-4.59984300	1.98780200
O	-0.31800300	-4.43863300	-2.86113100
O	-3.70648500	-0.06811800	0.27837800
O	-2.74310500	-2.48234800	0.49359300
O	-1.96265800	-2.40807400	-2.02079300
O	-0.39628500	-3.30669900	-0.18429400
O	0.41288700	-1.73327300	-3.41680400
O	0.61360700	-3.24542500	2.21762600
O	1.78577700	-3.12668600	-1.60478300

O	-0.10509100	-0.38409100	-1.29583400
O	3.94939500	-1.96053300	-0.36510500
C	4.39667800	-2.94490700	-2.91480800
H	2.49383100	-4.18817900	4.56682500
H	2.62259300	-2.63680000	5.43158200
H	1.09757500	-3.53693300	5.43754500
H	5.25014200	-2.26718100	-3.03194400
H	4.74455700	-3.89519300	-2.49684300
H	4.00976500	-3.15104600	-3.91896500
H	5.39748900	2.24296100	2.34434400
H	5.65511900	3.24976700	0.89367800
H	4.86000700	3.92290500	2.32249800
Os	3.39036200	-0.98328900	1.09953300
C	6.40558600	-2.15778800	0.30172700
C	6.43415700	-0.76383800	0.70424600
H	6.61714300	-2.91965000	1.04780900
H	6.11866300	-2.47945600	-0.69344000
H	7.26299300	-0.51028400	1.37453000
C	6.25126300	0.26875700	-0.37696000
H	6.09232600	1.26190000	0.04826900
H	7.16651700	0.30927800	-0.97837500
H	5.41431800	0.03706700	-1.04462200

### IM1<sub>A</sub>

W	-3.13287700	0.67282300	1.66414100
W	-0.16503100	2.73699400	2.45888400
W	-0.42053400	-0.82694100	3.43286100
Si	2.40113200	-2.35123200	2.57536400
P	0.30296700	0.05159800	0.03122300
O	-4.59525200	1.09424800	2.40905000
O	-0.45631100	3.79727400	3.75099600
O	-0.50880100	-1.10634200	5.10669800
O	-3.24043800	1.49523500	-0.05570300
O	-1.92230900	2.09453700	2.09946700
O	-2.21693700	-0.33797500	3.03452000
O	0.05686200	1.02398100	3.30707200
O	-0.65888800	-2.64124000	2.74899900
O	1.80269000	2.93078800	2.35165300
O	1.52151100	-1.10540800	3.10730900
O	-0.53609400	-0.77281600	1.00663600
O	1.77936200	-0.70646300	0.03105700
O	3.74323300	-1.54242600	1.68670800
O	5.71575600	0.04181800	0.76397000
C	3.34553500	-3.30366300	3.83822800



W	-3.02765600	-1.93182700	-0.85826800
W	-0.31654100	-3.42485900	1.03095000
W	0.12396200	-2.51971200	-2.56416100
Si	3.06060100	-1.03334100	-2.74806900
O	-4.41482700	-2.82270000	-1.25181500
O	-0.44368500	-5.09543500	1.30168500
O	0.16216400	-3.86410700	-3.59865300
O	-3.52877500	-0.92985100	0.69065600
O	-2.05618200	-3.07802500	0.33555400
O	-1.73652100	-2.43556200	-2.19919900
O	0.26659700	-3.21096900	-0.77600300
O	0.17179400	-1.02516400	-3.75772600
O	1.61384700	-3.21778000	1.46924300
O	2.09130800	-2.25881500	-2.36552100
O	-0.22635600	-0.15082200	-1.38733800
O	4.12315900	-0.78552800	-1.31090600
C	4.32812400	-1.38179600	-4.04239100
W	-2.69033600	1.53164100	-1.88591200
W	0.45006300	0.89337100	-3.45136900
W	0.24002800	3.58099900	-0.91660700
Si	2.79412200	3.10455700	1.08939500
O	-3.96540600	2.32356400	-2.67244200
O	0.77241500	1.41761900	-5.03535600
O	0.18935700	5.13330300	-1.59909000
O	-3.20498300	-0.30414100	-1.86543600
O	-1.41816800	1.23092600	-3.31240600
O	-1.50023000	2.93418900	-1.32038300
O	0.76922500	2.44625800	-2.38900300
O	-0.24892600	3.90081800	0.91971800
O	2.27792800	0.37472600	-2.85224700
O	2.12022100	3.58860900	-0.29567300
O	0.52968100	1.50238400	0.42995800
O	3.43165700	1.45838300	0.74533200
C	4.37948800	3.96114800	1.48194000
H	5.02813300	-0.54843200	-4.15826200
H	4.89258800	-2.29056800	-3.81191700
H	3.83039500	-1.53468500	-5.00611400
H	4.18543300	5.00610700	1.74502900
H	4.88635900	3.48911000	2.32915100
H	5.05033700	3.95475500	0.61682400
H	3.97350000	-2.64431900	4.44487000
H	2.64523300	-3.81201100	4.50982800
H	3.97752300	-4.06621500	3.37326000
Os	3.58616300	-0.29201800	0.36749700

C	6.74058800	-0.89971600	0.28011700
C	6.64740700	0.44712800	-0.27695300
H	6.29306400	-1.69296700	-0.32089900
H	7.32007800	1.22896500	0.07033200
H	6.18540900	0.59306600	-1.25203600
C	7.73888600	-1.29828300	1.30894700
H	8.09347000	-0.43310400	1.87661100
H	7.30729900	-2.02354500	2.00613400
H	8.59843700	-1.77127300	0.82181100

**IM1<sub>B</sub>**

W	-3.01912100	1.96938300	0.33317500
W	0.26089300	3.49075300	1.11953400
W	-1.26929400	0.86809600	3.22892400
Si	1.02886000	-1.44363900	3.84722200
P	0.25999100	-0.01942100	0.11823500
O	-4.36546800	2.99521900	0.39563900
O	0.11250400	5.05323600	1.76422800
O	-1.71187200	1.36307700	4.79286600
O	-2.54787100	1.93919000	-1.51460300
O	-1.51293000	3.14829500	0.52927100
O	-2.73276500	1.51119400	2.19073300
O	-0.22950600	2.34027900	2.57867000
O	-1.93817400	-0.96559200	3.23552700
O	2.17109400	3.18015500	1.53065100
O	0.52013500	0.06386400	3.56116200
O	-0.97494900	-0.08044800	1.01745900
O	1.35439000	-1.02430300	0.86350400
O	2.69610400	-1.42228100	3.14940400
O	5.22523100	-0.84651300	2.16994400
C	1.38917900	-1.89595200	5.59545200
W	-3.32896400	-1.41774200	-0.89094800
W	-1.58307800	-2.48305500	2.11420900
W	-0.29758600	-3.39639500	-1.26880600
Si	2.94479700	-2.85016800	-1.13228600
O	-4.83161100	-2.08327900	-1.30280600
O	-2.28734100	-3.78931000	2.93591000
O	-0.54862400	-5.02541400	-1.67192700
O	-3.76422500	0.24176600	-0.04587400
O	-2.97078300	-2.09269400	0.87005900
O	-2.05101400	-2.72747200	-1.50976700
O	-0.66463900	-3.22214000	0.61149000
O	0.44248300	-2.61696200	-2.85251100
O	0.20356800	-2.53073300	2.98907200

O	1.58671600	-3.55997600	-0.64869200
O	-0.05671700	-0.70639600	-1.20931100
O	3.73052300	-2.26375900	0.37043000
C	4.25689800	-3.96600000	-1.79386100
W	-1.71078900	1.04991500	-2.98632700
W	1.27322200	-0.87576800	-3.20581600
W	1.50974300	2.63180000	-2.04102200
Si	3.36406500	2.54810000	0.64758900
O	-2.49711000	1.68909700	-4.34404300
O	2.03128100	-1.19234600	-4.69412300
O	2.06140800	3.68673000	-3.25016700
O	-2.80828700	-0.41663700	-2.44240300
O	-0.38301400	-0.11880400	-3.76817600
O	-0.24909100	2.25086900	-2.64923600
O	1.89116900	0.87134600	-2.75486400
O	0.83351500	3.82972300	-0.70005200
O	2.69673300	-1.47020100	-1.93723100
O	3.17106800	2.53040900	-0.95684900
O	0.90292100	1.35580700	-0.00345600
O	3.44831700	0.81458100	1.08467500
C	5.02706200	3.13009000	1.20448400
H	3.92989500	-4.38758800	-2.75060100
H	5.19432100	-3.42917400	-1.97404200
H	4.45213300	-4.80044900	-1.11306600
H	5.05175600	4.22463800	1.17408300
H	5.22486800	2.82614400	2.23780700
H	5.83629000	2.76634500	0.56349500
H	0.45672200	-1.90089400	6.17031400
H	1.83213300	-2.89401200	5.66347200
H	2.06903400	-1.17552100	6.05961900
Os	3.14470000	-0.91764600	1.45985700
C	6.22907200	-1.86545300	1.92159500
C	6.39813200	-0.54423900	1.32011000
H	5.87440300	-2.67931900	1.28899400
H	6.76105800	-2.14497800	2.82776600
H	7.03125100	0.16393000	1.85446000
C	6.19641900	-0.28915700	-0.13616300
H	7.17918000	-0.26208500	-0.62006800
H	5.60461400	-1.07057100	-0.61924100
H	5.71438000	0.67545800	-0.32298500
<b>IM2 (s=1)</b>			
W	-2.92354300	0.01452300	-1.95578800
W	-0.16990200	-2.37036400	-2.69225100

W	0.14322900	1.25688600	-3.41009800
Si	3.07212000	2.21067200	-2.17815000
P	0.30617000	-0.08723300	0.02928500
O	-4.33190200	-0.06546200	-2.89504200
O	-0.42545200	-3.23177100	-4.13120700
O	0.11558900	1.64677500	-5.06174600
O	-3.38214900	-0.95011500	-0.38926200
O	-1.84254000	-1.50624200	-2.44290600
O	-1.69990300	0.99193500	-3.10971500
O	0.41855200	-0.63602200	-3.32113000
O	0.13739700	2.99796500	-2.50776300
O	1.73550300	-2.88230700	-2.35360700
O	2.13849600	1.37923800	-3.17641200
O	0.00528200	0.98227200	-1.00775800
O	1.85671500	0.29206800	0.60693400
O	3.90907700	0.72406500	-1.32012500
C	4.55481900	3.05514900	-2.85125700
W	-2.67523000	2.27144600	-0.90386300
W	0.40101800	3.42910800	-0.65546700
W	0.36439500	2.20282800	2.88958100
Si	2.96163200	0.14557800	3.08271300
O	-3.92359600	3.37051900	1.21927000
O	0.64122100	5.10780000	-0.71108300
O	0.46289000	3.44813600	4.03441100
O	-3.09722200	1.53792700	-0.83869000
O	-1.39001100	3.33228700	-0.12333300
O	-1.48244500	2.47198300	2.35589900
O	0.79088400	2.92007700	1.18487100
O	-0.09706900	0.60160300	3.84850100
O	2.31637300	2.84708100	-0.91814900
O	2.22486600	1.59374100	3.00775700
O	-0.51172400	0.08885300	1.30239800
O	4.00823100	-0.11645600	1.67746200
C	4.19709600	0.00531200	4.44260000
W	-3.06384900	-1.26335300	1.48183200
W	-0.06683800	-1.28564100	3.40713700
W	-0.39424800	-3.64801700	0.56255800
Si	2.46163000	-3.57105700	-1.08641200
O	-4.52264200	-1.92926500	2.02495200
O	-0.01915900	-2.00498000	4.94229100
O	-0.78905500	-5.22657700	1.03896500
O	-3.31919500	0.63256500	1.64608400
O	-1.95047400	-1.32488300	3.03969700
O	-2.05071400	-2.76692300	0.82837700

O	0.10912000	-2.75869300	2.18890900
O	-0.63319700	-3.68412700	-1.35656500
O	1.84240200	-1.03651100	3.02867500
O	1.53506000	-3.94578700	0.17096000
O	0.40462300	-1.51090100	-0.48904200
O	3.48877300	-2.16624600	-0.38766900
C	3.81177900	-4.75200100	-1.48029300
H	4.70008800	-0.96609500	4.42394100
H	4.95625200	0.78963300	4.36904200
H	3.69435900	0.10991800	5.40994000
H	3.38811900	-5.67697300	-1.88507700
H	4.49502200	-4.33998200	-2.22834400
H	4.38008000	-5.00821900	-0.58128200
H	5.10174500	2.39561500	-3.53140300
H	4.25804700	3.94773100	-3.41137800
H	5.22296800	3.37010800	-2.04429200
Os	3.43456200	-0.42363800	-0.07687300

**IM2 (s=3)**

W	-2.88992500	0.06676600	-1.99048300
W	-0.23114600	-2.41173300	-2.72963200
W	0.19597000	1.21575900	-3.33153000
Si	3.12990400	2.09069800	-2.00065900
P	0.26831100	-0.11936200	0.02296500
O	-4.31056700	-0.03920700	-2.90562400
O	-0.54080000	-3.27714100	-4.15429100
O	0.34935300	1.67779500	-4.95736700
O	-3.31224400	-0.89815400	-0.39411100
O	-1.87558300	-1.50229600	-2.45525200
O	-1.69222200	1.01774900	-3.17455900
O	0.35624800	-0.68957100	-3.36501600
O	0.19218000	2.95151200	-2.43235600
O	1.66162500	-2.93526200	-2.43921200
O	2.10808100	1.12034200	-2.78904400
O	-0.28027300	0.89562400	-0.96819200
O	1.84024100	0.45986100	0.30441000
O	4.11891300	0.86959800	-1.07758300
C	4.45071600	2.93006600	-2.96614600
W	-2.66185100	2.30295400	0.85032800
W	0.45993200	3.48236800	-0.61058100
W	0.34286700	2.18034400	2.88911300
Si	2.92813500	0.13215300	3.17633100
O	-3.90234000	3.39714400	1.20885500
O	0.64314600	5.16505700	-0.69197800

O	0.48976700	3.38472200	4.07298800
O	-3.14628300	1.59542900	-0.86933800
O	-1.36452200	3.36109600	-0.11531800
O	-1.45615900	2.45883400	2.34828000
O	0.80508400	2.98521400	1.21581800
O	-0.02339400	0.57371700	3.87334800
O	2.37090300	2.97000000	-0.88309100
O	2.24109800	1.55965000	2.88353700
O	-0.40443600	0.03922400	1.37864700
O	4.03183500	-0.17058600	1.76139100
C	4.11912100	0.04257700	4.57375100
W	-3.02547600	-1.24237300	1.45824700
W	-0.05581200	-1.31782400	3.40137200
W	-0.36432300	-3.65649400	0.54863400
Si	2.45619500	-3.51755100	-1.15991800
O	-4.49923300	-1.88943100	1.98336500
O	0.01651700	-2.03415800	4.93864200
O	-0.74661300	-5.23894900	1.02177900
O	-3.25019800	0.65819900	1.63073200
O	-1.92551800	-1.32291300	3.05108200
O	-2.01754800	-2.76026300	0.84073700
O	0.13405700	-2.79081600	2.19601400
O	-0.66901100	-3.69503200	-1.35560200
O	1.87721800	-1.07986600	2.98356300
O	1.56061300	-3.92002900	0.11949100
O	0.43557400	-1.53715300	-0.48449000
O	3.45634000	-2.07567600	-0.56549500
C	3.83188900	-4.67097100	-1.55425700
H	4.62908600	-0.92508600	4.59310800
H	4.86938900	0.83541700	4.50231400
H	3.58592100	0.16490900	5.52259900
H	3.42251300	-5.60677100	-1.94897200
H	4.49691300	-4.24875400	-2.31311900
H	4.41706500	-4.90981500	-0.66161200
H	5.00530100	2.21347900	-3.57909000
H	4.00516900	3.67553100	-3.63321400
H	5.15252900	3.44508100	-2.30363700
Os	3.47388000	-0.40007900	0.04866500

**AD2 (s=1)**

W	3.07964600	-1.44043400	-1.41932200
W	0.18423800	-0.70677300	-3.62265600
W	0.08879900	-3.39484700	-1.08183300
Si	-2.71388100	-3.08497400	0.67581500

P	-0.28577000	0.00799800	-0.04552500
O	4.47034100	-2.06105000	-2.16084600
O	0.45755500	-1.29362900	-5.18907100
O	0.00410700	-4.96616400	-1.71951200
O	3.44965600	0.43071800	-1.25888000
O	1.90484400	-0.91668800	-2.84347400
O	1.93622900	-2.99936500	-1.27385700
O	-0.25738500	-2.27198700	-2.59749600
O	0.27405200	-3.78994800	0.83009300
O	-1.74191900	-0.27647700	-3.79930300
O	-1.83179200	-3.05151400	-0.67276700
O	0.38029500	-1.34793500	0.15297000
O	-1.82966000	-0.13057400	0.58859500
O	-3.88192500	-1.72556300	0.44187800
O	-5.52785700	-0.13351600	-0.40249500
C	-3.90650000	-4.47328000	0.88299400
W	3.04098900	-0.60314300	2.11678700
W	0.08274300	-2.68332500	2.38063100
W	0.03719400	0.87885700	3.49800100
Si	-2.76618200	2.19709500	2.35222900
O	4.40577500	-0.88581300	3.07898400
O	0.06872300	-3.79149400	3.66416600
O	0.01682700	1.06388200	5.18398900
O	3.43601700	-1.47896000	0.45000000
O	1.89179000	-2.10844900	2.45474900
O	1.86920300	0.41686200	3.24113600
O	-0.31029000	-0.96486500	3.15353600
O	0.20511400	2.67150100	2.83684800
O	-1.86716800	-2.67714300	1.98135500
O	-1.92241700	1.10016500	3.17576800
O	0.35498800	1.03089600	0.88935400
O	-3.93394000	1.18936500	1.38748500
C	-3.92633500	3.24728200	3.31677500
W	3.03972000	2.06363100	-0.35243900
W	0.02180900	3.42757400	1.04107800
W	0.12905300	2.64302000	-2.57938700
Si	-2.60714400	0.98257000	-3.28052200
O	4.41189000	3.02373600	-0.60722200
O	-0.07507700	5.08536800	1.39453400
O	0.35406100	4.02382100	-3.53553700
O	3.41603000	1.04625400	1.22093300
O	1.87315300	3.22807200	0.66741500
O	1.86269100	2.42767700	-1.81508300
O	-0.32270000	3.33965500	-0.84088700

O	0.47629200	1.19718900	-3.80071400
O	-1.89706900	2.90521100	1.19208900
O	-1.79263700	2.33149400	-2.94068000
O	-0.42944000	0.45131900	-1.49492800
O	-3.15267200	0.38681100	-1.65238600
C	-4.21376400	1.23014700	-4.14062700
H	-3.35436700	3.93060600	3.95377600
H	-4.55740000	3.84697200	2.65446200
H	-4.56639000	2.63832300	3.96144300
H	-4.02916000	1.47059200	-5.19308700
H	-4.82659400	0.32462100	-4.10523200
H	-4.77368200	2.05697400	-3.69451600
H	-3.35421100	-5.40706100	1.03373700
H	-4.54546900	-4.30888800	1.75538800
H	-4.53749400	-4.58552900	-0.00318100
Os	-3.61831300	0.02750600	0.03393400
O	-5.41358600	1.13345200	-0.71335200

**AD2 (s=3)**

W	3.07643800	-1.44155900	-1.41972600
W	0.18675600	-0.69854000	-3.63193700
W	0.06876000	-3.38089600	-1.08136700
Si	-2.72147200	-3.08287000	0.69385000
P	-0.28266900	0.02812400	-0.04841100
O	4.46223900	-2.07297900	-2.16209800
O	0.47236200	-1.29208400	-5.19350000
O	-0.01829900	-4.95171700	-1.72026700
O	3.45216900	0.42822300	-1.26427100
O	1.90052400	-0.91494900	-2.84153400
O	1.91768800	-2.98979300	-1.26790100
O	-0.27213100	-2.25562900	-2.59473100
O	0.25465500	-3.77647700	0.83138800
O	-1.73207000	-0.26471600	-3.82880500
O	-1.85300300	-3.03904600	-0.66375100
O	0.35876000	-1.33762300	0.15684000
O	-1.83359900	-0.13742800	0.61951600
O	-3.90019600	-1.71940700	0.45133600
O	-5.64693600	-0.22246100	-0.80837300
C	-3.90702200	-4.47426300	0.91091200
W	3.04542700	-0.60086700	2.11666300
W	0.08089800	-2.67138200	2.38652500
W	0.04987500	0.89012500	3.51431900
Si	-2.75650300	2.18430400	2.35678800
O	4.41233000	-0.88892500	3.07467900



O	0.06512100	-3.78426800	3.66629600
O	0.04715700	1.07493800	5.20031500
O	3.43231800	-1.47957200	0.44694200
O	1.89249300	-2.10755300	2.44867400
O	1.88154500	0.41615000	3.24306000
O	-0.29895900	-0.95729700	3.16888900
O	0.23414000	2.67603000	2.84512800
O	-1.87464100	-2.65344000	1.99180900
O	-1.89963200	1.11213700	3.20122200
O	0.36080600	1.03958800	0.89184700
O	-3.91321800	1.20685800	1.37868200
C	-3.91430800	3.24003200	3.32098900
W	3.04637400	2.06386700	-0.35816200
W	0.03700300	3.43121600	1.04895200
W	0.12869700	2.64786400	-2.57567900
Si	-2.60355500	0.97568500	-3.27216700
O	4.42060100	3.02034300	-0.61626200
O	-0.05919200	5.08924400	1.40219700
O	0.34942500	4.03067800	-3.53022500
O	3.42288000	1.04466300	1.21540000
O	1.88696700	3.23129300	0.66546200
O	1.86687100	2.43039000	-1.81671200
O	-0.31401900	3.34384900	-0.83468600
O	0.48243400	1.20446800	-3.80131600
O	-1.87453400	2.90288800	1.20903500
O	-1.79159300	2.32949300	-2.93354100
O	-0.42923900	0.46681400	-1.49499200
O	-3.13191600	0.33989900	-1.68118800
C	-4.21655600	1.23480200	-4.12190700
H	-3.33976800	3.91704700	3.96242000
H	-4.54137200	3.84721900	2.66181600
H	-4.55954500	2.63354100	3.96312000
H	-4.04314400	1.54520700	-5.15783700
H	-4.80470200	0.31208700	-4.14325500
H	-4.80085700	2.01924800	-3.63113000
H	-3.35086700	-5.40582100	1.06181500
H	-4.54232100	-4.31224100	1.78655500
H	-4.54196500	-4.59471300	0.02854000
Os	-3.59368600	0.01876300	0.03232800
O	-5.47659000	1.02926800	-0.65246800

**AD2 (s=5)**

W	3.06469700	-1.46287400	-1.41035200
W	0.15643800	-0.70447600	-3.58819200

W	0.09600800	-3.40858000	-1.06518200
Si	-2.70870100	-3.11784000	0.70811700
P	-0.15255100	0.02946400	-0.04251800
O	4.45685200	-2.05691000	-2.16996300
O	0.37932200	-1.28082100	-5.16711100
O	-0.01522100	-4.98547000	-1.68493900
O	3.40745300	0.41251500	-1.24800300
O	1.88348400	-0.93716500	-2.84015600
O	1.95116000	-3.04133900	-1.27770700
O	-0.25972300	-2.29411400	-2.57302900
O	0.28898900	-3.77421700	0.85090600
O	-1.78254900	-0.29346100	-3.67120200
O	-1.81091100	-3.02911300	-0.63202700
O	0.52878600	-1.32168400	0.12917100
O	-1.67155900	-0.21897700	0.66275300
O	-3.87680300	-1.74967100	0.45539500
O	-5.96801600	0.10238600	-0.38619200
C	-3.86904400	-4.53423800	0.88373100
W	3.06497300	-0.62019200	2.11452400
W	0.09313200	-2.68044800	2.40835500
W	0.07657400	0.89637600	3.50567500
Si	-2.73124600	2.20004200	2.33743800
O	4.42864700	-0.90391600	3.07792600
O	0.08980700	-3.77911900	3.69976200
O	0.05826400	1.07478100	5.19192700
O	3.47019800	-1.49961400	0.45249700
O	1.90931700	-2.11504500	2.46802200
O	1.89744400	0.40593100	3.24763000
O	-0.28976400	-0.95159000	3.14393300
O	0.26266900	2.68435100	2.84706300
O	-1.86192300	-2.70677600	2.01533100
O	-1.87774400	1.12108200	3.17564000
O	0.47936500	1.06354200	0.87837200
O	-3.87750300	1.20637000	1.33770900
C	-3.90941200	3.24710300	3.28585700
W	3.04854600	2.05643700	-0.34086400
W	0.07465200	3.45755300	1.05744500
W	0.13236700	2.64502800	-2.55490100
Si	-2.63976600	0.99405600	-3.21266000
O	4.43844600	2.98264400	-0.62305000
O	-0.02782500	5.11219500	1.42379000
O	0.33560100	4.01489100	-3.53250400
O	3.44453500	1.03604200	1.22580700
O	1.92748800	3.26788700	0.67280700

O	1.87141200	2.43404300	-1.81239100
O	-0.28102900	3.37710000	-0.81925900
O	0.44331000	1.19448600	-3.78731700
O	-1.83646300	2.91879500	1.20174000
O	-1.80151700	2.32689600	-2.85739500
O	-0.40551200	0.47023100	-1.47021600
O	-3.41941200	0.49637800	-1.63519700
C	-4.17339700	1.28928400	-4.18807100
H	-3.34817600	3.93324100	3.92935500
H	-4.53593200	3.84617800	2.61866000
H	-4.55474200	2.63742100	3.92476300
H	-3.91286900	1.59586700	-5.20644300
H	-4.77854000	0.37999300	-4.25720000
H	-4.77720000	2.08579700	-3.74200800
H	-3.30109600	-5.46281700	1.00532000
H	-4.50681000	-4.41081600	1.76400300
H	-4.50439900	-4.63864300	-0.00060200
Os	-3.42885600	-0.02779000	0.08151000
O	-6.41009100	0.90915800	-1.18017100

**AD3 (s=1)**

W	3.14876400	-1.68821400	0.99165800
W	-0.04527000	-3.56400100	0.95339100
W	0.63803400	-0.90476300	3.43726200
Si	-1.97968100	1.14793700	3.52010000
P	-0.27127900	0.02786200	0.10765200
O	4.54991800	-2.55547900	1.38830800
O	0.16222600	-5.12738500	1.57805500
O	0.79241000	-1.46787000	5.03255500
O	3.17014700	-1.65021800	-0.92560700
O	1.76175700	-2.99414500	0.78925300
O	2.34719200	-1.33619100	2.71743700
O	-0.06487300	-2.42555600	2.49916100
O	1.11070700	0.98326300	3.67898500
O	-2.02706500	-3.53921700	0.91181900
O	-1.25033300	-0.29170800	3.44044800
O	0.65855200	0.19777900	1.30754900
O	-1.67063400	0.81299500	0.49744700
O	-3.41044100	0.98919200	2.45745100
O	-5.40875800	0.28213400	1.19748300
C	-2.82367500	1.55673800	5.10841000
W	3.33052800	1.78995800	-0.05255500
W	0.86740500	2.49011200	2.52346500
W	0.27008000	3.45297100	-1.03248800

Si	-2.84178300	2.57492800	-1.71616900
O	4.82108600	2.59519100	-0.08155700
O	1.21067300	3.81623200	3.52492800
O	0.38509400	5.12239700	-1.31748100
O	3.70832800	0.12401400	0.83109700
O	2.53230200	2.32334500	1.61038200
O	2.11726500	3.00550500	-0.91290600
O	0.25153200	3.23700100	0.85784600
O	0.02025000	2.70620900	-2.78982900
O	-1.06940300	2.32575000	2.90181200
O	-1.71205500	3.33702500	-0.85991100
O	0.28272100	0.83536800	-1.06860200
O	-3.89500600	1.79982900	-0.46783600
C	-4.06792500	3.64235400	-2.58060900
W	2.55465500	-0.77502300	-2.50447400
W	-0.49353700	0.91984600	-3.37194000
W	-0.64085600	-2.64759900	-2.37776600
Si	-3.05449200	-2.95956100	-0.18576700
O	3.68029200	-1.23757500	-3.68387200
O	-0.86811500	1.19814900	-5.00573700
O	-0.80508500	-3.68319600	-3.71117900
O	3.28866100	0.78886100	-1.68629800
O	1.30167900	0.32107500	-3.50172500
O	1.17897800	-2.10537300	-2.54813900
O	-1.02421800	-0.90590600	-3.08701600
O	-0.14946500	-3.85119700	-0.95134100
O	-2.26120000	1.31146000	-2.53332700
O	-2.49771500	-2.77103700	-1.68547000
O	-0.62823300	-1.42059600	-0.21588500
O	-3.31751700	-1.28667600	0.43158700
C	-4.76195000	-3.64593500	-0.08675800
H	-4.49162200	4.38722100	-1.90079300
H	-3.57641900	4.17485600	-3.40176300
H	-4.88063500	3.04439100	-3.00400000
H	-5.40773500	-3.17267400	-0.83249900
H	-4.74249200	-4.72232100	-0.28678300
H	-5.19240100	-3.49499400	0.90803500
H	-2.07087500	1.68668000	5.89324200
H	-3.39087100	2.48812400	5.02264900
H	-3.50293500	0.75568600	5.41357900
Os	-3.52389600	0.46529400	0.70422100
O	-5.64117700	-0.12249000	-0.04104900
C	-7.95153900	-0.97901800	-0.18328200
C	-8.22908500	0.34084600	-0.31534200

H	-7.87284500	-1.44550400	0.79781200
H	-7.82792800	-1.62494500	-1.04849800
H	-8.30568400	0.75466800	-1.32282700
C	-8.41185400	1.28065300	0.80812900
H	-7.68051200	2.09949000	0.74671800
H	-9.39786800	1.76274700	0.75701300
H	-8.31011100	0.79412300	1.78282100

**AD3 (s=3)**

W	3.00590600	-1.25246200	-1.40161500
W	0.11607200	-0.63199100	-3.63192900
W	0.10290700	-3.34380900	-1.11032300
Si	-2.73346100	-3.19197500	0.60978500
P	-0.45605900	0.03118300	-0.02375700
O	4.43891400	-1.79236700	-2.12714800
O	0.43532500	-1.18081400	-5.20392900
O	0.10658300	-4.91151900	-1.76294000
O	3.26386000	0.64275300	-1.22386400
O	1.83903400	-0.77130000	-2.84666800
O	1.94190400	-2.85571800	-1.27331900
O	-0.25778800	-2.22810000	-2.62269700
O	0.29937600	-3.74980400	0.79637700
O	-1.83162900	-0.32982400	-3.82507800
O	-1.82403400	-3.09720900	-0.72303600
O	0.27665800	-1.29539100	0.16723800
O	-1.98627100	-0.22553100	0.57668300
O	-3.98852200	-1.93294800	0.36483900
O	-6.03875500	-0.32149900	0.26236700
C	-3.79939100	-4.68357800	0.78369500
W	2.88828500	-0.44843900	2.14314200
W	0.02738200	-2.66935200	2.35331800
W	-0.18794800	0.87153000	3.51814200
Si	-3.04557300	2.04421700	2.35786600
O	4.25901300	-0.67470400	3.11262900
O	0.05991400	-3.79444200	3.62263400
O	-0.22918200	1.03563700	5.20632000
O	3.34809800	-1.27536900	0.46965900
O	1.81304100	-2.00833200	2.45184900
O	1.66609000	0.50201700	3.27302300
O	-0.44136300	-0.98717200	3.15742500
O	-0.09075100	2.68678300	2.88667800
O	-1.91311000	-2.75618900	1.92906400
O	-2.13803000	0.99155700	3.17084200
O	0.13459700	1.07448200	0.92233200

O	-4.13740100	1.06157400	1.34882800
C	-4.22839400	3.01137600	3.39352900
W	2.77578500	2.23640100	-0.30320600
W	-0.30208600	3.44963900	1.10546100
W	-0.16161900	2.68355300	-2.51950300
Si	-2.77888300	0.84069100	-3.25199100
O	4.10290300	3.26305800	-0.54001000
O	-0.46515400	5.10429300	1.45582800
O	-0.03460000	4.09098800	-3.45735100
O	3.18671800	1.23284300	1.26615700
O	1.54704800	3.34371800	0.71624200
O	1.58352000	2.57522500	-1.76763300
O	-0.67082000	3.33442600	-0.78348500
O	0.28681000	1.28468300	-3.77250100
O	-2.20727100	2.88528100	1.26253800
O	-2.06980800	2.25316400	-2.91753300
O	-0.56373000	0.47387100	-1.47889600
O	-3.19891200	0.17984400	-1.64247900
C	-4.41177700	0.95908600	-4.10094900
H	-3.70227200	3.37154000	4.28461000
H	-4.61300800	3.88768200	2.86224500
H	-5.07235500	2.40081100	3.72931000
H	-4.28876300	1.40923500	-5.09157400
H	-4.84198200	-0.03810900	-4.23736500
H	-5.12627400	1.56991600	-3.54008400
H	-3.16665400	-5.56941600	0.90643200
H	-4.44706400	-4.60492700	1.66165100
H	-4.42327800	-4.83216100	-0.10252900
Os	-3.79503300	-0.14593200	0.00927300
O	-5.65684700	0.04166400	-0.92275000
C	-5.90818600	2.80405300	-0.90171700
C	-4.60218700	3.11662700	-1.09219600
H	-6.52677500	2.59145900	-1.77730500
H	-4.16498500	3.19726800	-2.08526900
H	-3.92841600	3.34049600	-0.26210000
C	-6.58521600	2.76246500	0.40835400
H	-7.54540500	3.29262100	0.37687200
H	-6.82951700	1.72256700	0.69199100
H	-5.96912100	3.18154900	1.20836000

**AD3 (s=5)**

W	-2.81951900	1.50111000	1.61917400
W	0.36295000	3.34070500	1.23665300
W	0.01840200	0.42025000	3.49773500

Si	2.56157700	-1.64846800	2.95622300
P	0.23176800	-0.06860000	-0.05640000
O	-4.12956900	2.33123300	2.30172100
O	0.36473000	4.82117800	2.06580600
O	0.16171400	0.78897600	5.14942400
O	-3.08672400	1.65382500	-0.26323300
O	-1.46811900	2.84608800	1.36788200
O	-1.78220500	0.94629100	3.15070100
O	0.60116500	2.01954400	2.61716400
O	-0.44473800	-1.47521700	3.57866800
O	2.30266300	3.24350500	0.83414900
O	1.86582600	-0.19812300	3.10214200
O	-0.45864800	-0.39336900	1.26503000
O	1.63626000	-0.97613400	0.00878800
O	3.78612600	-1.35553800	1.66238600
O	5.83318200	-0.48100100	0.07653900
C	3.64062900	-2.20849300	4.33907500
W	-3.28428800	-1.81942900	0.22997100
W	-0.43356800	-2.84677300	2.23235200
W	-0.47339500	-3.37531300	-1.46667700
Si	2.49778600	-2.41652800	-2.54574700
O	-4.77192600	-2.61920200	0.36496700
O	-0.63897400	-4.28769300	3.10365600
O	-0.70029000	-4.99793100	-1.90478100
O	-3.47117000	-0.27900700	1.35360100
O	-2.22010000	-2.55855400	1.65809300
O	-2.24982500	-2.93210000	-0.94974300
O	-0.10111700	-3.35117700	0.41169100
O	-0.51828500	-2.41469700	-3.12314700
O	1.55274100	-2.74227700	2.34314800
O	1.51139400	-3.32466000	-1.65176000
O	-0.53862500	-0.69298800	-1.21647700
O	3.76144200	-1.79350400	-1.41025500
C	3.54326400	-3.30847200	-3.77029400
W	-2.86208600	0.97625700	-2.03737900
W	-0.06146400	-0.56811400	-3.59221100
W	0.31246500	2.86069700	-2.23847400
Si	3.10328100	2.82523900	-0.50254200
O	-4.18750000	1.59612300	-2.89115600
O	0.06640500	-0.69616000	-5.28104100
O	0.28805400	4.06193000	-3.43608100
O	-3.51236000	-0.65212300	-1.27459400
O	-1.86378500	0.02649400	-3.38905700
O	-1.51170500	2.33935100	-2.19040800

O	0.51919200	1.21293200	-3.22918200
O	0.12768700	3.87129400	-0.60832100
O	1.78423500	-1.04930200	-3.03216000
O	2.26291400	2.83721000	-1.87912700
O	0.61705300	1.38725800	-0.25157300
O	3.56364200	1.10134000	-0.23732700
C	4.79341400	3.55282800	-0.63817000
H	2.91152700	-3.70465900	-4.57261400
H	4.28315900	-2.64016500	-4.22046100
H	4.06454000	-4.14959700	-3.30394600
H	4.72919700	4.64253400	-0.72184800
H	5.39311900	3.31760500	0.24735000
H	5.31063400	3.17585700	-1.52623000
H	3.02599800	-2.42163600	5.22020000
H	4.17929200	-3.12335800	4.07487800
H	4.36699800	-1.43770900	4.61394000
Os	3.48560300	-0.67724700	0.00057300
O	6.35480800	0.31483900	-0.71871800
C	8.29188100	1.16058000	1.23293300
C	8.83475100	1.11510100	-0.00005100
H	7.95147100	2.12442900	1.61887700
H	8.94541800	2.00736200	-0.61160200
H	9.20783900	0.18153500	-0.41943600
C	8.08232900	-0.01505600	2.10299800
H	7.00532000	-0.18580000	2.26716400
H	8.50714200	-0.92980800	1.67707500
H	8.50957400	0.14253800	3.10199500

**TS2 (s=1)**

W	3.11840400	-1.66601100	0.99735900
W	-0.05714800	-3.56553700	0.94143400
W	0.59734600	-0.90001800	3.42347000
Si	-2.03572100	1.14000000	3.49184700
P	-0.30695400	0.02933700	0.09984400
O	4.52351000	-2.53153400	1.38476100
O	0.15713000	-5.13041800	1.56177100
O	0.74228000	-1.45583700	5.02281900
O	3.13004400	-1.62690700	-0.92275400
O	1.74313000	-2.98763000	0.78395000
O	2.32079800	-1.33206900	2.72227200
O	-0.08727500	-2.43118400	2.49061600
O	1.06949200	0.98723700	3.66341500
O	-2.04172400	-3.55410500	0.90944200
O	-1.28456000	-0.29219200	3.40486100



O	0.66047800	0.18328400	1.27671300
O	-1.69038900	0.77255400	0.55904000
O	-3.47807300	0.97830300	2.46852400
O	-5.46003400	0.26250700	1.14464600
C	-2.84426600	1.52444800	5.10675200
W	3.28810800	1.80711200	-0.04331800
W	0.81219000	2.50092600	2.52229500
W	0.22734700	3.46088000	-1.03593500
Si	-2.87835100	2.56876000	-1.71072300
O	4.77385800	2.62197800	-0.07568500
O	1.15728000	3.82374900	3.52800700
O	0.33732000	5.13083200	-1.32298200
O	3.68654600	0.14371700	0.83516400
O	2.48614100	2.34023200	1.61086900
O	2.07077200	3.01718500	-0.91394100
O	0.20686900	3.25326200	0.85724300
O	-0.02623000	2.71741700	-2.79536100
O	-1.11571400	2.33017200	2.90399700
O	-1.75397400	3.33823900	-0.85720400
O	0.23105000	0.84413300	-1.08085300
O	-3.92029900	1.78371100	-0.46327200
C	-4.11251100	3.63407800	-2.56906800
W	2.51974600	-0.75520000	-2.50165600
W	-0.53040600	0.92779400	-3.37381900
W	-0.66760600	-2.63880100	-2.38337300
Si	-3.06732200	-2.96595600	-0.18242300
O	3.65273000	-1.21246700	-3.67672200
O	-0.90914400	1.20641800	-5.00767000
O	-0.83583800	-3.67388900	-3.71786100
O	3.24521900	0.80954100	-1.68177300
O	1.26497100	0.33458100	-3.50688000
O	1.14928500	-2.09391900	-2.55767600
O	-1.05922900	-0.90071000	-3.09394500
O	-0.17039600	-3.84899500	-0.96316100
O	-2.30231200	1.30946200	-2.53537000
O	-2.52718600	-2.77059800	-1.68671200
O	-0.65768400	-1.42335600	-0.22936700
O	-3.35556600	-1.30887000	0.45439100
C	-4.77121800	-3.67074700	-0.08424000
H	-4.53756800	4.37574000	-1.88642000
H	-3.62511000	4.17211100	-3.38907700
H	-4.92366300	3.03561800	-2.99502500
H	-5.40060100	-3.26439900	-0.88185800
H	-4.73063300	-4.75789600	-0.20837700

H	-5.23267900	-3.46100600	0.88621100
H	-2.07273800	1.64935300	5.87411400
H	-3.41967000	2.45306000	5.04882700
H	-3.51086500	0.71584100	5.42011400
Os	-3.56878000	0.44342400	0.70198400
O	-5.81453900	-0.15337800	-0.10064100
C	-7.57527500	-0.88052600	-0.06836800
C	-8.16787800	0.35766400	-0.27740900
H	-7.52576500	-1.30487400	0.93215000
H	-7.43891800	-1.57185100	-0.89496400
H	-8.31605800	0.68537100	-1.30749700
C	-8.48491000	1.30455500	0.79382700
H	-7.82518900	2.18443300	0.71461500
H	-9.50115100	1.70643800	0.67523900
H	-8.37250000	0.87715200	1.79356900

**TS2 (s=3)**

W	-3.44946400	0.97331200	0.83706900
W	-0.77176200	3.53377800	0.89917000
W	-0.92044800	0.81216900	3.41010100
Si	2.07922500	-0.57259200	3.65066800
P	0.34203400	0.08624900	0.12702700
O	-5.02569000	1.49094000	1.18523000
O	-1.35281600	5.01410300	1.48929900
O	-1.30447800	1.34526500	4.97695800
O	-3.38814100	0.90630800	-1.07171000
O	-2.40264200	2.56752800	0.68014000
O	-2.63107900	0.79831900	2.58172500
O	-0.55414900	2.44438000	2.46666400
O	-0.94473000	-1.12894100	3.67778900
O	1.15825200	3.95698000	0.92696200
O	1.06092700	0.67179400	3.54474700
O	-0.48796300	-0.30120100	1.34632000
O	1.90572300	-0.36809200	0.44822600
O	3.46075400	-0.10833800	2.58756500
O	5.42527800	0.91525200	1.52043000
C	2.96971200	-0.77212700	5.25132300
W	-2.77754900	-2.46485000	-0.14722000
W	-0.32208600	-2.54203000	2.53793000
W	0.62923000	-3.40410900	-0.96350300
Si	3.46998100	-1.82121400	-1.52416200
O	-4.03263100	-3.60277400	-0.19997100
O	-0.39522500	-3.90055400	3.55242900
O	0.87552900	-5.06229600	-1.23001900

O	-3.55956100	-0.92444500	0.69046700
O	-1.93251900	-2.75577700	1.56205000
O	-1.27816000	-3.37136300	-0.91500600
O	0.52886600	-3.16850800	0.92222300
O	0.74516600	-2.61731400	-2.71592800
O	1.51754500	-1.92391800	2.98281100
O	2.52988300	-2.87254700	-0.74576700
O	-0.02787700	-0.82684100	-1.04528900
O	4.30708200	-0.82654400	-0.30755500
C	4.90985700	-2.59694900	-2.38703000
W	-2.51713900	0.17666500	-2.61199800
W	0.87231500	-0.76913900	-3.31152100
W	0.14300300	2.74697000	-2.38933900
Si	2.33923400	3.61718600	-0.12019800
O	-3.66640800	0.36148500	-3.84398100
O	1.38062900	-0.97182200	-4.92041300
O	0.10844400	3.77269400	-3.74017200
O	-2.91852600	-1.51146100	-1.80045600
O	-1.00897200	-0.60431700	-3.53840600
O	-1.49163900	1.79041100	-2.61481000
O	0.95203200	1.13174500	-3.04562600
O	-0.66656700	3.81840600	-1.00802500
O	2.63609900	-0.74251700	-2.39083800
O	1.89025800	3.30570000	-1.63928300
O	0.32768300	1.57497500	-0.20003600
O	2.96092300	2.05940700	0.50318200
C	3.82351500	4.69829300	0.03491700
H	4.53760600	-3.19063700	-3.22961100
H	5.60661200	-1.85686900	-2.79456800
H	5.45775800	-3.27639500	-1.72628000
H	3.56095800	5.72989000	-0.22153200
H	4.20792300	4.69262600	1.05948500
H	4.61878600	4.37175700	-0.64196500
H	2.25340800	-1.05670500	6.02965100
H	3.72918900	-1.55642000	5.18558900
H	3.44956500	0.16275200	5.55510700
Os	3.58655400	0.41753100	0.85476300
O	5.51468600	1.46186000	0.27038200
C	7.72164900	0.00186500	0.11961500
C	6.87314300	0.67794000	-0.77167200
H	8.53506900	0.56603100	0.57900400
H	7.17813800	1.64134100	-1.17316800
H	6.20065600	0.09555000	-1.39802200
C	7.50833700	-1.38434400	0.56302000

H	6.70848800	-1.88430000	0.00994100
H	8.43236400	-1.97344100	0.48853500
H	7.24018200	-1.39524000	1.63158700

**TS2 (s=5)**

W	-2.77052400	1.09033300	2.11286100
W	0.35183800	3.07961900	1.93170400
W	0.20791300	-0.24846200	3.54740200
Si	2.73881200	-2.08364000	2.42685500
P	0.24622700	-0.00050500	-0.03045000
O	-4.03477500	1.71510200	3.05316800
O	0.35783200	4.35594100	3.05031300
O	0.45087400	-0.24594700	5.22997600
O	-3.20971400	1.65882300	0.33470600
O	-1.45112400	2.48662600	2.03735300
O	-1.62409500	0.26766700	3.43073900
O	0.69246500	1.51699500	3.01954400
O	-0.21831900	-2.13971000	3.24531200
O	2.26997900	3.09604400	1.43722500
O	2.03516500	-0.71115700	2.90803100
O	-0.39273900	-0.57161500	1.23479600
O	1.67308100	-0.82911300	-0.18097500
O	3.89906400	-1.51890400	1.17330400
O	5.73296900	-0.38783600	-0.43902100
C	3.87845400	-2.90135900	3.62211300
W	-3.24821700	-1.86698600	0.06048100
W	-0.27028600	-3.20238400	1.65539700
W	-0.51776900	-2.95046100	-2.06136000
Si	2.35581000	-1.67968500	-3.07760400
O	-4.71502500	-2.71484800	0.09992700
O	-0.39974200	-4.79318900	2.23130700
O	-0.72588700	-4.44670800	-2.83554900
O	-3.39854500	-0.60066100	1.50160800
O	-2.09197700	-2.85323300	1.24273600
O	-2.27782900	-2.68526700	-1.38122600
O	-0.05033100	-3.34061800	-0.24991400
O	-0.68382300	-1.66728200	-3.48087500
O	1.71368800	-3.06116900	1.65824300
O	1.44542900	-2.77345100	-2.32096800
O	-0.57179500	-0.43169300	-1.24744700
O	3.68622500	-1.29038600	-1.92771700
C	3.31153700	-2.28548200	-4.53160100
W	-3.02247800	1.38212900	-1.54061800
W	-0.30154900	0.24443700	-3.56227000

W	0.12965900	3.32061500	-1.55330100
Si	3.00378200	3.00612500	0.00157100
O	-4.39644300	2.12399700	-2.19996000
O	-0.29323600	0.48544700	-5.24466200
O	-0.00082900	4.74039700	-2.47370400
O	-3.57198400	-0.40700100	-1.13082500
O	-2.07639800	0.74388500	-3.10943900
O	-1.69030300	2.75801200	-1.47251500
O	0.29037100	1.93450400	-2.86937900
O	0.02088600	3.97890700	0.26446700
O	1.59761300	-0.26312600	-3.23989900
O	2.09306800	3.30503800	-1.29853000
O	0.57268500	1.48469100	0.03129200
O	3.53046000	1.29706900	-0.16496400
C	4.64084000	3.85843400	-0.03495500
H	2.61950300	-2.53929600	-5.34193500
H	3.99783500	-1.51855000	-4.90281900
H	3.88502800	-3.18355400	-4.28400400
H	4.49076800	4.93991100	0.04843200
H	5.26831800	3.54125000	0.80384300
H	5.16947400	3.66463200	-0.97354000
H	3.30167900	-3.27959500	4.47307800
H	4.39255700	-3.74989700	3.16098500
H	4.62451300	-2.19974000	4.00658400
Os	3.52858200	-0.49880500	-0.29291400
O	6.21815600	0.80330900	-0.25906400
C	8.50874700	-0.21743300	0.40714000
C	7.95193300	0.76888800	-0.44830300
H	8.75895900	0.07635300	1.42714400
H	8.09740800	1.81739600	-0.19136600
H	7.96592500	0.56897600	-1.52044600
C	8.64019000	-1.63897200	0.03461200
H	7.93844700	-2.25721400	0.61575300
H	8.43935800	-1.81580200	-1.02642600
H	9.64046800	-2.02231800	0.27623700

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W	2.76634900	-1.77706000	0.55780700
W	-0.41931400	-3.60272900	1.05669200
W	0.70498700	-0.98144200	3.42214600
Si	-1.73931700	1.19514200	3.98979500
P	-0.71722300	0.04208600	0.26930800
O	4.19030100	-2.68312100	0.71329000
O	-0.12979800	-5.17918300	1.60888200

O	1.15903000	-1.59227200	4.93965900
O	2.41860200	-1.71606800	-1.32772600
O	1.34174400	-3.06455600	0.60690600
O	2.24932600	-1.38437900	2.37145400
O	-0.16463600	-2.46239100	2.60736400
O	1.30498900	0.88867600	3.61568200
O	-2.35692500	-3.54692500	1.40196500
O	-1.11676300	-0.28462500	3.84881500
O	0.26070800	0.24355400	1.42834800
O	-2.09240600	0.80656900	0.66674000
O	-3.30296300	1.11739100	3.04254700
O	-5.53185900	0.32742200	1.90802300
C	-2.42389200	1.64808400	5.63471600
W	2.89504000	1.70623200	-0.49516600
W	0.95239100	2.40255800	2.51632900
W	-0.19015900	3.55602400	-0.84330800
Si	-3.40926600	2.82639200	-0.93734700
O	4.39098400	2.46136400	-0.74624300
O	1.52920100	3.68674000	3.46346000
O	-0.00469100	5.21792200	-1.12937000
O	3.35050000	0.00915200	0.29503700
O	2.39737700	2.18067700	1.31096300
O	1.62589500	2.99908800	-1.07938900
O	0.09391800	3.25491800	0.99642900
O	-0.74146000	2.79747300	-2.52412500
O	-0.92274200	2.33189700	3.20235400
O	-2.11329800	3.58732700	-0.36234600
O	-0.18410700	0.76987800	-0.96983300
O	-4.23125900	2.07388900	0.46026100
C	-4.73121800	3.94502200	-1.57139100
W	1.58896800	-0.77955000	-2.76617000
W	-1.44572300	1.05773300	-3.02336800
W	-1.58942900	-2.52603200	-2.03619300
Si	-3.53760200	-2.76504600	0.61977700
O	2.46626300	-1.29021000	-4.12150100
O	-2.14740600	1.37735500	-4.53984900
O	-2.11470100	-3.49356500	-3.33033500
O	2.55535300	0.73885500	-2.11302700
O	0.23581400	0.37193300	-3.55375700
O	0.16408400	-2.05974600	-2.59593000
O	-2.03700600	-0.72846200	-2.62024500
O	-0.88761200	-3.83331800	-0.80202500
O	-3.01370900	1.57611600	-1.87932800
O	-3.26570400	-2.56089700	-0.96364700

O	-1.05173200	-1.43427900	0.03719200
O	-3.41665800	-1.20295200	1.46645400
C	-5.23623900	-3.34761300	1.04119300
H	-5.09410200	4.61337000	-0.78434900
H	-4.32490500	4.56718800	-2.37621600
H	-5.58453600	3.39244200	-1.97791900
H	-5.99854700	-2.72778200	0.56004000
H	-5.36539300	-4.38154200	0.70309400
H	-5.39872800	-3.32418100	2.12320500
H	-1.60753300	1.76245800	6.35572000
H	-2.96677000	2.59647900	5.58252300
H	-3.10012500	0.87363800	6.00831000
Os	-3.88010600	0.55123400	1.43208400
O	-4.99308900	-0.44772100	-0.47366600
C	-5.10953900	-0.52863700	-1.91592700
C	-6.12763000	0.17400300	-1.13785700
H	-5.29118300	-1.55387300	-2.23630500
H	-4.35141200	0.02511300	-2.45863900
H	-6.05164900	1.26444500	-1.11315400
C	-7.46297300	-0.40280300	-0.80700000
H	-7.76706900	-0.13557800	0.21055400
H	-8.21733000	-0.00927200	-1.49702300
H	-7.45752600	-1.49388600	-0.89809400